

A. P. Smith, H. Ade (NCSU), S. G. Urquhart, A. P. Hitchcock (McMaster U.) and E. G. Rightor (Dow Chemical).

Due to the dependence of Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy on the local chemical environment of the excited atom<sup>1</sup>, differences in these absorption spectra might also be expected for different isomers of the same material. In order to investigate this phenomenon, we have acquired carbon K-edge absorption spectra of poly(diallyl phthalate) (1,2 PDP), poly(diallyl isophthalate) (1,3 PDP), and poly(ethylene terephthalate) (1,4 PET), where the phthalate segment of these polymers are isomers with different patterns of substitution (ortho, meta, para) of the methyl carboxylate groups on the phenyl ring. Fig. 1 displays the chemical structure of these materials and Fig. 2 shows the x-ray absorption spectra of a) 1,4 PET, b) 1,3 PDP and c) 1,2 PDP and demonstrates that while the spectra are similar in overall shape, there are differences. The most obvious difference between the spectra is the split in the  $\pi^*$  peak at 285 eV present in the 1,4 PET and absent in the other oligimers. This peak intensity splitting has been shown to be due to the conjugation between the carbonyl groups and the aromatic group<sup>2</sup> which is absent in the oligimers due to differences in electronic structure (1,3 PDP) and non-planar geometry (1,2 PDP)<sup>3</sup>. In addition, the absolute energy of the peaks at 285 and 288 eV shift upwards by .3 eV between the 1,4 PET and the 1,2 PDP spectra. These spectra demonstrate that NEXAFS spectroscopy can be quite sensitive to isomer substitution in conjugated moieties.

[1] J. Stöhr. *NEXAFS Spectroscopy*, Springer-Verlag (Berlin), 1992.

[2] E. G. Rightor *et al.* *J. Phys. Chem.* (in press)

[3] S. G. Urquhart *et. al.* *J. Phys. Chem.* (submitted)

Work supported by NSF Young Investigator Award (DMR-9458060) and Dow Chemical.

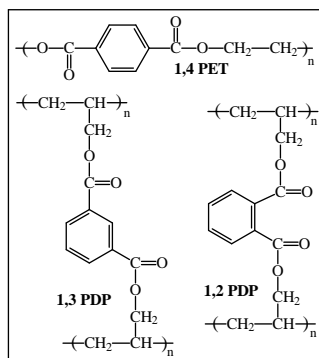


Figure 1. Chemical formulas of 1,4 PET, 1,3 PDP, and 1,2 PDP.

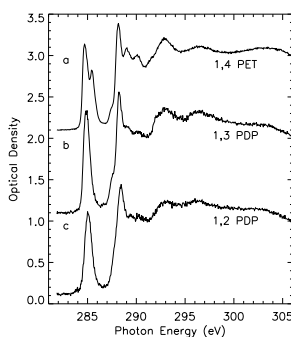


Figure 2. NEXAFS spectra of 1,4 PET, 1,3 PDP, and 1,2 PDP demonstrating changes due to chemical isomerism.